

**UNITED STATES  
ENVIRONMENTAL PROTECTION AGENCY (EPA)  
HIGH PRODUCTION VOLUME (HPV)  
CHEMICAL CHALLENGE PROGRAM**

**ROBUST SUMMARIES DOSSIER**

**for**

**C9 MEMBERS**

**of the**

**HIGHER OLEFINS CATEGORY**

**Members containing C9 olefins:**

CAS No. 27215-95-8, Nonene  
CAS No. 68526-55-6; Alkenes, C8-10, C9-Rich  
CAS No. 68526-54-5, Alkenes, C7-9, C8-Rich\*  
CAS No. 68526-56-7; Alkenes, C9-11, C10-Rich\*

\*Addressed in the C8 and C10 dossiers

**Contains Robust Summaries for the Following Substances:**

CAS No. 27215-95-8, Nonene  
CAS No. 124-11-8, 1-Nonene/Isononene  
CAS No. 68526-54-5, Alkenes, C7-9, C8-Rich  
CAS No. 68526-55-6; Alkenes, C8-10, C9-Rich  
CAS No. 68526-56-7; Alkenes, C9-11, C10-Rich

**Prepared by:**

**American Chemistry Council  
Higher Olefins Panel**

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## 1. GENERAL INFORMATION

### 1.01 Details on Chemical Category

The Higher Olefins Category consists of a non-continuous range of odd- and even-numbered mono-unsaturated linear and branched olefins (C<sub>6</sub> through C<sub>54</sub>) under 30 CAS numbers, 13 for alpha olefins and 17 for internal olefins. All CAS numbers are within the HPV Challenge Program. The C<sub>6</sub> – C<sub>14</sub> even-numbered linear alpha olefins were sponsored under the OECD SIDS program (SIAM 11). The Panel sponsored the C<sub>6</sub>, C<sub>7</sub>, C<sub>8</sub>, C<sub>9</sub>, C<sub>10</sub>, C<sub>12</sub> and C<sub>10-13</sub> aliphatic linear and branched internal olefins and the C<sub>16</sub> and C<sub>18</sub> aliphatic linear alpha olefins in the OECD HPV Chemicals Programme (SIAM 19). The members of the category are presented below.

#### Members of the Higher Olefins Category

Alpha Olefins	Branched/Linear	CAS No.
Neohexene	Branched	558-37-2
1-Tridecene	Linear	2437-56-1
1-Hexadecene (ICCA)	Linear	629-73-2
1-Octadecene (ICCA)	Linear	112-88-9
1-Eicosene	Linear	3452-07-1
1-Docosene	Linear	1599-67-3
1-Tetracosene	Linear	10192-32-2
Alkenes, C10-16 alpha	Linear	68855-58-3
Alkenes, C14-18 alpha	Linear	68855-59-4
Alkenes, C14-20 alpha	Linear	68855-60-7
a-Olefin fraction C20-24 cut	Linear	93924-10-8
a-Olefin fraction C24-28 cut	Branched and Linear	93924-11-9
Alkene, C24-54 branched and linear, alpha	Branched and Linear	131459-42-2
<b>Internal Olefins</b>		
Hexene (ICCA)	Linear	25264-93-1
Heptene (ICCA)	Linear	25339-56-4
Octene (ICCA)	Linear	25377-83-7
Nonene (ICCA)	Linear	27215-95-8
Dodecene (ICCA – not sponsored in HPV)	Linear	25378-22-7
Alkenes, C6	Branched and Linear	68526-52-3
Alkenes, C6-8, C7 rich	No data available	68526-53-4
Alkenes, C7-9, C8-rich	Linear	68526-54-5
Alkenes, C8-10, C9-rich	Linear	68526-55-6
Alkenes, C9-11, C10-rich	Linear	68526-56-7
Alkenes, C10-12, C11-rich	Linear	68526-57-8
Alkenes, C11-13, C12-rich	Linear	68526-58-9
Heavy polymerization naphtha (petroleum)	Branched	68783-10-8
Alkenes, C10-16	Linear	68991-52-6
Alkenes, C15-C18	Linear	93762-80-2
C10,12 Olefin rich hydrocarbons	Linear	68514-32-9
C12,14 Olefin rich hydrocarbons	Linear	68514-33-0

## 1.1 General Substance Information

### A. Type of Substance

Element [ ]; Inorganic [ ]; Natural substance [ ]; Organic [X ]; Organometallic [ ];  
Petroleum product [ ]

### B. Physical State (at 20°C and 1.013 hPa)

Gaseous [ ]; Liquid [X ]; Solid [ ]

C. Purity: No data for nonene; other C9 containing category members are  
manufactured and marketed as blends

## 1.2 Impurities

Remark: The compositions reported by manufacturers are shown below:

Nonene	27215-95-8	nda
Alkenes, C8-10, C9- rich	68526-55-6	Mostly linear, less than 2% branched. Typical composition: 1% C8 olefins, 91% C9 olefins, 8% C10 olefins.

## 1.3 Additives

None

## 1.4 Synonyms

Some synonyms are: Nonene (mixed isomers)  
Propylene trimer  
Nonenes  
Tripropylene

## 1.5 Quantity

Remarks: A Chemical Economics Handbook marketing report indicated that 2000 global  
production for nonene was approximately 1037 million pounds (470,000 metric  
tons) with the United States accounting for almost 56% (SRI, 2001). Range of  
U.S. production volumes for 2002 submitted by Higher Olefin Panel members to  
Panel Manager: CAS No. 27215-95-8, Nonene = 100-200 million pounds;  
CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich = 300-400 million pounds

Reference: American Chemistry Council's Higher Olefins Panel (2002)

## 1.6 Use Pattern

## **A. General Use Pattern**

### **Type of Use:**

### **Category:**

(a) Main  
Industrial  
Use

Use in closed systems  
Chemical industry – chemicals used in synthesis  
Intermediate

### **Remarks:**

Intermediate in the manufacture of plasticizer alcohols and surfactants

(b) Main  
Industrial  
Use

Non-dispersive use  
Chemical industry – chemicals used in synthesis  
Intermediate

### **Remarks:**

Intermediate in the manufacture of plasticizer alcohols and surfactants

Reference: American Chemistry Council's Higher Olefins Panel (2002)

## **B. Uses In Consumer Products**

Not applicable

## **1.7 Sources of Exposure**

### **Source:**

Remarks: These products are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals. No non-intermediate applications have been identified. Any occupational exposures that do occur are most likely by the inhalation and dermal routes. It is a common practice to use personal protective equipment. In the case of dermal exposures, protective gloves would be worn due to the mildly irritating properties of this class of chemicals (ACC Higher Olefins Panel). Results from modelled data suggest that on-site waste treatment processes are expected to remove these substances from aqueous waste streams to the extent that they will not be readily detectable in effluent discharge (EPIWIN, 2000). These substances are not on the US Toxic Release Inventory (TRI) list (NLM, 2003). These olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes.

Reference: American Chemistry Council's Higher Olefins Panel (2002)

## **1.8 Additional Information**

### **A. Classification and Labelling**

### **B. Occupational Exposure Limits**

## **Exposure Limit Value**

Type: None available  
Value:

## **Short Term Exposure Limit Value**

Value: None available  
Length of  
exposure period:  
Frequency:

### **C. Options for Disposal**

Remarks: Incineration, diversion to other hydrocarbon uses

### **D. Last Literature Search**

Type of search: Internal and external  
Date of search: October 2003  
Remark: Medline  
IUCLID  
TSCATS  
ChemIDplus  
AQUIRE - ECOTOX

## **2. PHYSICAL CHEMICAL DATA**

### **2.1 Melting Point**

#### **A. Test Substance**

Identity: CAS No. 27215-95-8, Nonene

#### **Method**

Method/  
guideline followed: Calculated value using MPBPWIN version 1.41, a subroutine of  
EPIWIN version 3.1

GLP: Not applicable  
Year: Not applicable

**Test Conditions:** Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula  $T_m = 0.5839T_b$ ,

where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Program used the structure for 2-nonene.

**Results**

Melting point  
value in °C: -56.70°C

**Reliability:** (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

Identity: CAS No. 27215-95-8, Nonene

**Method**

Method/guideline followed: No data  
GLP: No data  
Year: No data

**Test Conditions:** No data

**Results**

Melting point value in °C: ca. -80 to -90 °C

**Reliability:** (4) Not assignable. These data were not reviewed for quality.

**References:** Enichem S.p.A Milan , manufacturer's data (cited in IUCLID)

**C. Test Substance**

Identity: CAS 124-11-8, 1-Nonene

**Method**

Method/guideline followed: No data  
GLP: No data  
Year: No data

**Test Conditions:** No data

**Results**

Melting point value in °C: -81.3 °C

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79<sup>th</sup> ed. Boca Raton, FL: CRC Press Inc., p. 3-225.

## 2.2 Boiling Point

### A. Test Substance

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method/  
guideline followed:** Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used the structure for 2-nonene.

**Results**

Boiling point  
value in °C: 149.53°C

Pressure: 1013

Pressure unit: hPa

**Reliability:** (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.  
EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method:** No data

**GLP:** No data

**Year:** No data

**Test Conditions:** No data

**Results**

**Boiling point value:** ca. 135 - 140°C

**Pressure:** 1013 hPa

**Remarks:**

**Reliability:** (4) Not assignable. These data were not reviewed for quality.

**References:** Enichem S.p.A Milan , manufacturer's data (cited in IUCLID);

**C. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method/guideline followed:** No data

**GLP:** No data

**Year:** No data

**Test Conditions:** No data

**Results**

**Boiling point value:** 135 – 140°C

**Pressure:** 1013 hPa

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** U.S. Coast Guard Department of Transportation. CHRIS – Chemical Hazards Response Information System Washington, DC, information last updated 2002, website: <http://www.chrismanual.com/default.htm>.



**D. Test Substance**

Identity: CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

**Method**

Method/  
guideline followed: Calculated value using MPBPWIN version 1.41, a subroutine of  
EPIWIN version 3.11

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Boiling Point is calculated by the MPBPWIN subroutine, which is based  
on the method of Stein and Brown (1994). Program used the structure  
for 1-nonene.

**Results**

Boiling point  
value in °C: 141.02°C

Pressure: 1013

Pressure unit: hPa

**Reliability:** (2) Reliable with restrictions. The result is calculated data based on  
chemical structure as modeled by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Stein, S. and R. Brown (1994) Estimation of normal boiling points from  
group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000). Estimation Program Interface for Windows, version  
3.11. EPI Suite™ software, U.S. Environmental Protection Agency,  
Office of Pollution Prevention and Toxics, U.S.A.

**E. Test Substance**

Identity: CAS No. 124-11-8, Isononene

**Method**

Method/guideline followed: No data

GLP: No data

Year: No data

**Test Conditions:** No data

**Results**

Boiling point value: 146.9°C

Pressure: 1013 hPa

**Reliability:** (2) Reliable with restrictions. The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A

## 2.3 Density

### A. Test Substance

**Identity:** CAS No. 27215-95-8, Nonene

#### Method

**Method:** No data  
**GLP:** No data

**Test Conditions:** No data

#### Results

**Type:** Density  
**Value:** ca. 0.74 – 0.747 g/cm<sup>3</sup>  
**Temperature (°C):** 15°C

**Reliability:** (4) Not assignable. These data were not reviewed for quality.

**Reference:** Enichem S.p.A Milan , manufacturer's data (cited in IUCLID)

### B. Test Substance

**Identity:** CAS No. 27215-95-8, Nonene

#### Method

**Method:** No data  
**GLP:** No data

**Test Conditions:** No data

#### Results

**Type:** Specific gravity  
**Value:** 0.739  
**Temperature (°C):** 20°C

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. These data were not reviewed for quality.

**Reference:** U.S. Coast Guard Department of Transportation. CHRIS – Chemical Hazards Response Information System Washington, DC, information last updated 2002, website: <http://www.chrismanual.com/default.htm>.

**C. Test Substance**

**Identity:** CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

**Method**

**Method:** No data

**GLP:** No data

**Test Conditions:** No data

**Results**

**Type:** Density

**Value:** ca. 0.75 g/cm<sup>3</sup>

**Temperature (°C):** 15°C

**Reliability:** (2) Reliable with restrictions. Reliable source. These data were not reviewed for quality.

**Reference:** ExxonMobil (2004) Nonene Datasheet (unpublished data)

**2.4 Vapour Pressure**

**A. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method/  
guideline followed:** Not reported

**GLP:** Not applicable

**Year:**

**Test Conditions:**

**Results**

**Vapor Pressure**

**Value:** 5.00 hPa

**Temperature:** 25°C

**Remarks:** Reported as 3.75 mm Hg (25°C)

**Reliability:** (2) Reliable with restrictions. The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Weber, R.C. et al. (1981) Vapor Pressure Distribution of Selected Organic Chemicals. USEPA -600/2-81-021, Cincinnati, OH: USEPA pp.39; EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

Method/  
guideline followed: Not reported  
GLP: Not applicable  
Year:

**Test Conditions:**

**Results**

Vapor Pressure  
Value: ca. 53.32 – 66.66 hPa  
Temperature: 50°C

**Reliability:** (4) Not assignable. These data were not reviewed for quality.

**References:** Enichem S.p.A Milan , manufacturer's data (cited in IUCLID)

**C. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41  
GLP: Not applicable  
Year: Not applicable

**Test Conditions:** Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described

by Neely and Blau, 1985. The calculation used a value for BP of 149.53 °C, estimated by EPIWIN using the structure for 2-nonene.

## Results

Vapor Pressure  
value: 6.98 hPa  
Temperature (°C): 25°C  
Remarks: Reported as 5.24 mm Hg

**Reliability:** (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN and estimated data from EPIWIN.

**References:** Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## D. Test Substance

Identity: CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

### Method

Method/  
guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used an experimental value for BP of 146.9 °C, cited in the EPIWIN database.

## Results

Vapor Pressure  
value: 7.85 hPa  
Temperature (°C): 25°C  
Remarks: Reported as 5.89 mm Hg

**Reliability:** (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals. Volume 1, p. 31, CRC Press.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### **E. Test Substance**

**Identity:** CAS No. 124-11-8, Isononene

#### **Method**

Method/  
guideline followed: Not reported  
GLP: Not applicable  
Year:

#### **Test Conditions:**

#### **Results**

Vapor Pressure  
Value: 7.20 hPa  
Temperature: 25°C  
Remarks: Reported as 5.4 mm Hg (25°C)

**Reliability:** (2) Reliable with restrictions. The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Daubert TE and Danner RP (1989) as cited in EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### **2.5 Partition Coefficient (log10Kow)**

#### **A. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method:** Calculated value using the computer program EPIWIN, KOWWIN v

1.67

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used the structure for 2-nonene.

**Results**

**Log Kow:** 4.55

**Temperature (°C):** Not applicable

**Reliability:** (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EPIWIN.

**Flag:** Key study for SIDS endpoint

**Reference:** Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

**Identity:** CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

**Method**

**Method:** Calculated value using the computer program EPIWIN, KOWWIN v

1.67

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used the structure for 1-nonene.

**Results**

Log Kow:	4.62
Temperature (°C):	Not applicable
<b>Reliability:</b>	(2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EPIWIN.
<b>Flag:</b>	Key study for SIDS endpoint
<b>Reference:</b>	Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. <i>J. Pharm. Sci.</i> 84:83-92.
	EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**C. Test Substance**

Identity: CAS No. 124-11-8, Isononene

**Method**

Method:	No data
GLP:	No data
Year:	No data

**Test Conditions:** No data

**Results**

Log Kow:	5.15
Temperature (°C):	No data

**Reliability:** (2) Reliable with restrictions. The result is experimental data as cited in the EPIWIN database. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**Reference:** Hansch C et al. (1995) as cited in EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**2.6.1 Water Solubility (including \*Dissociation Constant).**

**A. Test Substance**

Identity: CAS No. 27215-95-8, Nonene



**Method**

Method/  
guideline followed:

Calculated value using the computer program EPIWIN,  
WSKOW v 1.41

GLP:

Not applicable

Year:

Not applicable

**Test Conditions:**

Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an estimated Log Kow of 4.55 (EPIWIN) which was estimated using the structure for 2-nonene.

**Results**

Value(mg/L) at  
temperature ( °C):

3.619 mg/L (25°C)

**Reliability:**

(2) Reliable with restrictions. The result was calculated using estimated data as modeled by EPIWIN.

**Flag:**

Key study for SIDS endpoint

**References:**

Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. Environ. Toxicol. Chem. 15:100-106.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

Identity:

CAS No. 27215-95-8, Nonene

**Method**

Method/  
guideline followed:

Calculated value using the computer program EPIWIN,  
WATERNT v 1.01

GLP:

Not applicable

Year:

Not applicable

**Test Conditions:**

The calculation was based on chemical structure as modeled by EPIWIN.

**Results**

Value(mg/L) at  
temperature ( °C):

2.7615 mg/L (25°C)

**Reliability:**

(2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EPIWIN.

**References:**

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**C. Test Substance**

Identity:

CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

**Method**

Method/  
guideline followed:

Calculated value using the computer program EPIWIN,  
WSKOW v 1.41

GLP:

Not applicable

Year:

Not applicable

**Test Conditions:**

Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an experimental Log Kow of 4.55 cited in the EPIWIN database.

**Results**

Value(mg/L) at  
temperature ( °C):

1.101 mg/L (25°C)

**Reliability:**

(2) Reliable with restrictions. The result was calculated.

**Flag:**

Key study for SIDS endpoint

**References:**

Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. Environ. Toxicol. Chem. 15:100-106.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**D. Test Substance**

Identity:

CAS No. 124-11-8, Isononene

**Method**

Method/  
guideline followed: No data  
GLP: No data  
Year: No data

**Test Conditions:** No data

**Results**

Value(mg/L) at  
temperature ( °C): 1.12 mg/L (25°C)

**Reliability:** (2) Reliable with restrictions. The result is experimental data as cited in the EPIWIN database. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Yalkowsky, SH and Dannenfelser RM (1992) as cited in EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**2.6.2 Surface tension**

No data available

**2.7 Flash Point (Liquids)****A. Test Substance**

Identity: CAS No. 27215-95-8, Nonene

**Method**

Method: No data  
GLP:

**Test Conditions:** No data

**Results**

Value (°C): 25.6 °C  
Type of test: Open cup

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. These data were not reviewed for quality.

**Reference:** U.S. Coast Guard Department of Transportation. CHRIS – Chemical Hazards Response Information System Washington, DC, information last updated 2002, website: <http://www.chrismanual.com/default.htm>.

**B. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method:** Directive 84/449/EEC, A.9 "Flash point"  
**Year:** 1985  
**GLP:**

**Test Conditions:** No data

**Results**

**Value (°C):** ca. range 20-23°C  
**Type of test:** Closed cup

**Reliability:** (4) Not assignable. These data were not reviewed for quality.

**Reference:** Enichem S.p.A Milan , manufacturer's data (cited in IUCLID)

**2.8 Auto Flammability (Solids/Gases)**

**Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method:** Directive 84/449EEC, A.15 "Auto-flammability of volatile liquids or gases"  
**GLP:** No data

**Test Conditions:** No data

**Results**

**Value (°C):** ca. 245 – 420 °C  
**Pressure (hPa):** No data

**Reliability** (4) Not assignable. These data were not reviewed for quality.

**Reference:** Enichem S.p.A Milan , manufacturer's data (cited in IUCLID)

## **2.9 Flammability**

### **Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

### **Method**

**Method:** No data

**GLP:** No data

**Test Conditions:** No data

**Result:** Highly flammable

**Lower flammability limit:** 0.7% in air (estimated)

**Upper flammability limit:** 3.9% in air (estimated)

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data were not evaluated for quality.

**Reference:** U.S. Coast Guard Department of Transportation. CHRIS – Chemical Hazards Response Information System Washington, DC, information last updated 2002, website: <http://www.chrismanual.com/default.htm>.

## **2.10 Explosive Properties**

No data available

## **2.11 Oxidising Properties**

No data available

## **2.12 Oxidation-Reduction Potential**

No data available

## **2.13 Additional Information**

# **3. ENVIRONMENTAL FATE AND PATHWAYS**

## **3.1 Stability**

## A. Photodegradation

### (1) Test Substance

Identity: CAS No. 27215-95-8, Nonene; or CAS No. 68526-55-6;  
Alkenes, C8-10, C9 Rich

#### Method

Method/  
guideline followed: Other: Technical discussion

Type: water  
GLP: Not applicable  
Year: Not applicable

Test Conditions: Not applicable

#### Results

Direct photolysis: In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Higher Olefins Category.

Remarks: The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982a). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982a). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982a). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Olefins with one double bond, such as the chemicals in the Higher Olefins category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerization about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (Harris, 1982a).

Products in the Higher Olefins Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

**Reliability:** Not applicable

**References:** Harris J C (1982a). Rate of Aqueous Photolysis. Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline (1977). Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

**(2) Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method/  
guideline followed:** Calculated values using AOPWIN version 1.91, a subroutine of the computer program EIPWIN version 3.11 which uses a program described by Meylan, W.M. and Howard, P.H. (1993). Program used the structure for 2-nonene.

**Type:** air  
**GLP:** Nor applicable  
**Year:** Not applicable

**Results**

Indirect photolysis

**Sensitiser (type):** OH  
**Rate Constant:**  $63.2401 \text{ E-12 cm}^3/\text{molecule-sec}$  (cis isomer)  
**Degradation % after:** 50% after 2.030 hrs (using 12-hr day and avg. OH conc. of  $1.5 \text{ E6 OH/cm}^3$ ) (cis isomer)

Rate Constant:	70.8401 E-12 cm <sup>3</sup> /molecule-sec (trans isomer)
Degradation % after:	50% after 1.812 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm <sup>3</sup> ) (trans isomer)
Sensitiser (type):	Ozone
Rate Constant:	13 E-17 cm <sup>3</sup> /molecule-sec (cis isomer)
Degradation % after:	50% after 2.116 hrs (using avg. ozone conc. of 7 E11 mol/cm <sup>3</sup> ) (Cis isomer)
Rate Constant:	20 E-17 cm <sup>3</sup> /molecule-sec (trans isomer)
Degradation % after:	50% after 1.375 hrs (using avg. ozone conc. of 7 E11 mol/cm <sup>3</sup> ) (trans isomer)
<b>Reliability:</b>	(2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust summary has a rating of 2 because the data are calculated and not measured.
<b>Flag:</b>	Critical study for SIDS endpoint
<b>References:</b>	Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. <i>Chemosphere</i> 26: 2293-99  EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## B. Stability in Water

### Test Substance

Identity: CAS No. 27215-95-8, Nonene; or CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

### Method

Method/  
guideline followed: Other – Technical Discussion

**Test Conditions:** Not applicable

**Results:** Not applicable

**Remarks:** Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H<sub>2</sub>O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982b). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is



the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond. The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (Harris, 1982b) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Higher Olefins Category, will react with water by an addition reaction mechanism (Gould, 1959). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (Harris, 1982b). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

The substances in the Higher Olefins Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Higher Olefins Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

**Conclusions:** In the environment, hydrolysis will not contribute to the degradation of C9 olefins.

**Reliability:** Not applicable

**References:** Gould, E.S. (1959) Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982b) "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

Neely, W. B. (1985) Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

## C. Stability In Soil

No data available

### 3.2 Monitoring Data (Environment)

No data available.

### 3.3 Transport and Distribution

#### 3.3.1 Transport between environmental compartments

##### A. Test Substance

Identity: CAS No. 27215-95-8, Nonene

##### Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

Chemical assumptions:

Molecular weight: 126  
Water solubility: 3.619 g/m<sup>3</sup>  
Vapor pressure: 500 Pa (25°C)  
Log Kow: 4.55  
Melting point: -56.7°C  
Environment name: EQC Standard Environment

Half-life in air = 1.4 hr, half-life in water = 208 hr, half-life in soil = 208 hr,  
half-life in sediment = 832 hr

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

**Results** Media: Air, soil, water and sediment concentrations were estimated

	Level I	Level III
<b>Air</b>	99%	<1%
<b>Water</b>	<1%	41.2%
<b>Soil</b>	<1%	52.6%
<b>Sediment</b>	<1%	5.2%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

**Conclusions:** These results indicated that nonene will partition primarily to air under equilibrium conditions (Level I model), but primarily to water and soil under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

**Reliability:** (2) Valid with restrictions: Data are calculated.

**Flag:** Critical study for SIDS endpoint

**References:** Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1.). Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at <http://www.trentu.ca/cemc>)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### **B. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

##### **Method**

**Type:** Volatilization from water

**Remarks:** Calculated values using AOPWIN version 1.90, a subroutine of the computer program EIPWIN version 3.11 which uses a program described by Meylan, W.M. and Howard, P.H. (1993) based on Henry's Law Constant of 0.99 atm-m<sup>3</sup>/mole (estimated by Bond SAR method using HENRYWIN program) and EPIWIN default values

**Results:** Half-life from a model river: 1.147 hrs  
Half-life from a model lake: 4.4 days

**Reliability:** (2) Valid with restrictions. Values are calculated.

**References:** Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 26: 2293-99

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### **3.3.2 Distribution**

##### **A. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method:** Adsorption Coefficient (Koc) calculated value using the computer program EPIWIN, PCKOC v 1.66, using the method described by Meylon et al., 1992.

**Test Conditions:** Based on chemical structure; program used the structure for 2-nonene.

**Results**

**Value:** Estimated Koc = 935

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** Meylan, W., P.H. Howard and R.S. Boethling (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. Environ. Sci. Technol. 26:1560-7

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

**Identity:** CAS No. 27215-95-8, Nonene

**Method**

**Method:** Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.10

**Test Conditions:** Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on EPIWIN values of VP = 5.24 mm Hg and WS = 3.62 mg/L. Program used the structure for 2-nonene.

**Results**

**Value:** Bond estimate =  $0.990 \text{ atm-m}^3/\text{mole}$   
Group estimate =  $1.04 \text{ atm-m}^3/\text{mole}$   
VP/Wsol estimate =  $0.2405 \text{ atm-m}^3/\text{mole}$

**Reliability:** (2) Reliable with restrictions. Values are calculated.

**Reference:** EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### 3.4 Aerobic Biodegradation

#### A. Test Substance

Identity: CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

#### Method

Method/guideline: OECD 301F, Ready Biodegradability, Manometric Respirometry Test

Type: Aerobic [X] Anaerobic [ ]

GLP: Yes

Year: 1995

Contact time: 28 days

Inoculum: Domestic activated sludge

**Test Conditions:** Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, and calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material loading was approximately 32 mg/L. [Reason for using 32 mg/L instead of 100 mg/L: Substances such as this test material typically have ThODs between 2 and 3 mg per mg substance. Thus, the test material concentration was adjusted for a target of 100 mg THOD/L] Sodium benzoate (positive control) concentration was approximately 44 mg/L. Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

**Results:** Approximately 29% biodegradation of the test material was measured on day 28. Approximately 10% biodegradation was achieved on day 17.

By day 14, >60% biodegradation of the positive control was measured, which meets the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

<u>Sample</u>	<u>% Degradation*</u> <u>(day 28)</u>	<u>Mean % Degradation</u> <u>(day 28)</u>
Test Material	44.1, 28.6, 15.0	29.2
Na Benzoate	98.9, 95.5	97.2

\* replicate data

**Reliability:** (2) Reliable with restrictions: The range in biodegradation values is not less than 20% as required in the OECD test guideline.

**Flag:** Key study for SIDS endpoint

**Reference:** Exxon Biomedical Sciences, Inc. (1997) Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119194A. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

## **B. Test Substance**

**Identity:** CAS No. 68526-56-7; Alkenes, C9-11, C10 Rich

### **Method**

**Method/guideline:** OECD 301F, Ready Biodegradability, Manometric Respirometry Test

**Type:** Aerobic [X] Anaerobic [ ]

**GLP:** Yes

**Year:** 1995

**Contact time:** 28 days

**Inoculum:** Domestic activated sludge

**Test Conditions:** Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, and calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material loading was approximately 42 mg/L. [Reason for using 42 mg/L instead of 100 mg/L: Substances such as this test material typically have ThODs between 2 and 3 mg per mg substance. Thus, the test material concentration was adjusted for a target of 100 mg THOD/L] Sodium benzoate (positive control) concentration was approximately 44 mg/L. Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

**Results:** Approximately 21% biodegradation of the test material was measured on day 28. Approximately 10% biodegradation was achieved on day 17.

By day 14, >60% biodegradation of the positive control was measured, which meets the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

<u>Sample</u>	<u>% Degradation*</u> <u>(day 28)</u>	<u>Mean % Degradation</u> <u>(day 28)</u>
Test Material	20.9, 19.9, 22.6	21.1
Na Benzoate	98.9, 95.5	97.2

\* replicate data

**Reliability:** (1) Reliable without restriction

**Flag:** Key study for SIDS endpoint

**Reference:** Exxon Biomedical Sciences, Inc. (1997) Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119294A. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

## C. Test Substance

**Identity:** CAS No. 27215-95-8, Nonene

### Method

**Method/guideline:** Estimated using the computer program EPIWIN v 3.10, BIOWIN v 4.01

**Type:** Aerobic

**Test Conditions:** Estimates use methods described by Howard et al., 1992; Boethling et al., 1994; and Tunkel et al., 2000. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

**Results:** Linear model prediction: Biodegrades fast  
Non-linear model prediction: Biodegrades fast  
Ultimate biodegradation timeframe: Days-Weeks  
Primary biodegradation timeframe: Days  
MITI linear model prediction: Biodegrades fast  
MITI non-linear model prediction: Biodegrades fast

**Reliability:** (2) Reliable with restriction: Results are estimated.

**Reference:** Boethling, R.S., P.H. Howard, W. Meylan, W. Stiteler, J. Beaumann and N. Tirado (1994) Group contribution method for predicting probability and rate of aerobic biodegradation. Environ. Sci. Technol. 28:459-65.

Howard, P.H., R.S. Boethling, W.M. Stiteler, W.M. Meylan, A.E. Hueber, J.A. Beauman and M.E. Larosche (1992) Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. Environ. Toxicol. Chem. 11:593-603.

Tunkel, J. P.H. Howard, R.S. Boethling, W. Stiteler and H. Loonen (2000) Predicting ready biodegradability in the MITI Test. Environ. Toxicol. Chem. (accepted for publication)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### **3.5 BOD5, COD or ratio BOD5/COD**

No data available

### **3.6 Bioaccumulation**

#### **Test Substance**

Identity: CAS No. 27215-95-8, Nonene

#### **Method**

Method: BCF calculated value using the computer program EPIWIN, BCF v 2.15

**Test Conditions:** Based on chemical structure and a Log Kow of 4.55 (estimated data from EPIWIN) using methods described by Meylan et al., 1999. Formula used to make BCF estimate:  $\text{Log BCF} = 0.77 \log \text{Kow} - 0.70$  with no correction factor.

#### **Results**

Value: Estimated Log BCF = 2.801 (BCF = 631.9)

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** Meylan,WM, Howard,PH, Boethling,RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### **3.7 Additional Information**

#### **A. Sewage Treatment**

##### **Test Substance**

Identity: CAS No. 27215-95-8, Nonene



**Test Method:** Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.

**Input values:** MW = 126.24; Henry's LC = 0.99 atm-m<sup>3</sup>/mol; air-water partition coefficient = 40.4881; Log Kow = 4.55; biomass to water partition coefficient = 7097.07; temperature = 25°C

**GLP:** No

**Test Medium:** Secondary waste water treatment (water)

**Test Type:** Aerobic

**Test Results:** 99.81 % removed from wastewater treatment

**Reference:** EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### 4. ENVIRONMENTAL TOXICITY

##### 4.1 Acute Toxicity to Fish

###### A. Test Substance

**Identity:** CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

###### Method

**Method/guideline:** OECD 203

**Test type:** Semistatic Fish Acute Toxicity Test

**GLP:** Yes [X] No [ ]

**Year:** 1995

**Species/Strain:** Rainbow Trout (*Oncorhynchus mykiss*)

**Analytical Monitoring:** Yes

**Exposure period:** 96 hours

**Statistical methods:** Trimmed Spearman-Kärber Method (Hamilton, M.A. *et al.* 1977. Trimmed Spearman-Kärber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719.)

**Test Conditions:** Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of <10%. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22°C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 4 fish were added. Three replicates of each test material

loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 2.6, 4.3, 7.2, 12, and 20 mg/L, which measured 0.2, 0.4, 0.7, 1.2, and 2.5 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions. A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.2 mg/L.

Water hardness was 174-178 mg/L as CaCO<sub>3</sub>. Test temperature was 15°C (sd = 0.09). Lighting was 578 to 580 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 8.5 to 10.2 mg/L for "new" solutions and 6.5 to 8.5 mg/L for "old" solutions. The pH ranged from 7.0 to 8.8 for "new" solutions and 7.0 to 8.4 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.272 g; mean total length at test termination = 3.5 cm; test loading = 0.24 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

**Results:**

96-hour LL50 = 8.9 mg/L (95% CI 9.9 to 13.3 mg/L) based upon loading rates.

96-hour LC50 = 0.87 mg/L (95% CI 0.79 to 0.96 mg/L) based upon measured values of old and new solutions.

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).

<u>Loading Rate (mg/L)</u>	<u>Measured Conc. (mg/L)</u>	<u>Fish Total Mortality (@96 hrs)*</u>
Control	Control	0
2.6	0.2	0
4.3	0.4	0
7.2	0.7	1
12	1.2	12
20	2.5	12

\* 12 fish added at test initiation

**Reliability:**

(1) Reliable without restriction

**Flag:**

Key study for SIDS endpoint

**References:**

Exxon Biomedical Sciences, Inc. (1996) Fish, Acute Toxicity Test. Study #119158. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

## B. Test Substance

Identity: CAS No. 68526-56-7; Alkenes, C9-11, C10 Rich

### Method

Method/guideline: OECD 203  
Test type: Semistatic Fish Acute Toxicity Test  
GLP: Yes [X] No [ ]  
Year: 1995  
Species/Strain: Rainbow Trout (*Oncorhynchus mykiss*)  
Analytical Monitoring: Yes  
Exposure period: 96 hours  
Statistical methods: Trimmed Spearman-Kärber Method (Hamilton, M.A. *et al.* 1977. Trimmed Spearman-Kärber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. *Environ. Sci. Technol.* 11:714-719.)

**Test Conditions:** Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of <10%. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22°C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 4 fish were added. Three replicates of each test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 0.2, 0.4, 1.2, 3.5, and 10 mg/L, which measured 0.01, 0.03, 0.06, 0.08, and 2.6 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions. A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.03 mg/L.

Water hardness was 160-180 mg/L as CaCO<sub>3</sub>. Test temperature was 16°C (sd = 0.2). Lighting was 445 to 555 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 8.7 to 9.9 mg/L for "new" solutions and 7.2 to 8.5 mg/L for "old" solutions. The pH ranged from 7.0 to 8.8 for "new" solutions and 7.3 to 8.7 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.175 g; mean total length at test termination = 3.0 cm; test loading = 0.19 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels

in the closed system. Fish size had no significant effect on study outcome.

**Results:** 96-hour LL50 = 4.8 mg/L (95% CI 3.8 to 6.0 mg/L) based upon loading rates.  
96-hour LC50 = 0.12 mg/L (95% CI 0.11 to 0.14 mg/L) based upon measured values of old and new solutions.

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).

<u>Loading Rate (mg/L)</u>	<u>Measured Conc. (mg/L)</u>	<u>Fish Total Mortality (@96 hrs)*</u>
Control	Control	0
0.2	0.01	0
0.4	0.03	0
1.2	0.06	0
3.5	0.08	3
10	0.26	15**

\* 15 fish added at test initiation

\*\* 1 mortality not test related

**Reliability:** (1) Reliable without restriction

**Flag:** Key study for SIDS endpoint

**References:** Exxon Biomedical Sciences, Inc. (1996) Fish, Acute Toxicity Test. Study #119258. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

## C. Test Substance

**Identity:** CAS No. 124-11-8, 1-Nonene

### Method

**Method/guideline:** 96 hour semistatic toxicity test

**Test type:** semistatic

**GLP:** No

**Year:** 1985

**Species/Strain:** *Brachydanio rerio* (zebra fish)

**Analytical Monitoring:** No

**Exposure period:** 96 hr

**Statistical methods:** The LL50 values were calculated by means of a parametric model developed by Kooijman [Kooijman, S.A.L.M. (1981) Parametric analyses of mortality rates in bioassays. Water Res. 15:105-119.]

**Test Conditions:** The test animals were 4-6 weeks old,  $3 \pm 1$  cm, born and grown in the laboratory in fresh-water. Necessary amounts of test material were

added to 1 L fresh water (pH ~8, hardness ~210 mg CaCO<sub>3</sub> per liter) in glass stoppered conical flasks and stirred for 4 hr before adding test animals (10/ flask). Test conditions: 24°C; no aeration, food, or replicate; test medium renewed daily. At none of the dose levels was test substance visible during the test period. pH and oxygen were monitored. The target for oxygen concentration was 70% of the saturation level. The concentrations tested: 0, 3.2, 10, and 32 mg/L (nominal).

<b>Results:</b>	<p>LL<sub>50</sub> (24 hr) estimated to be about 11 mg/L (LL0 = 3.2 mg/L, LL100 = 32 mg/L)          LL<sub>50</sub> (48 hr) estimated to be about 6 mg/L (LL0 = 3.2 mg/L, LL100 = 10 mg/L)          LL<sub>50</sub> (72 hr) &lt; 3.2 mg/L (LL0 &lt; 3.2 mg/L)          LL<sub>50</sub> (96 hr) &lt; 3.2 mg/L (LL0 &lt; 3.2 mg/L)</p> <p>NOEC (96 hr) &lt; 3.2 mg/L (nominal)</p>
<b>Remarks:</b>	Assessment of condition of test animals compared to the controls was by visual estimation.
<b>Reliability:</b>	(2) Reliable with restrictions. Study does not totally comply with current testing guidelines. No chemical analyses were performed.
<b>References:</b>	Adema, D.M.M. and Bakker, G.H. (1985) Aquatic toxicity of compounds that may be carried by ships [MARPOL 1973; Annex II]. TNO report R 85/217, The Hague (unpublished report).

## 4.2 Acute Toxicity to Aquatic Invertebrates (e.g. Daphnia)

### Test Substance

Identity: CAS No. 124-11-8, 1-Nonene

### Method

Method/guideline: 48-hr static toxicity test  
 Test type: Static  
 GLP: No  
 Year: 1985  
 Analytical Monitoring: No  
 Species/Strain: *Daphnia magna*  
 Exposure period: 48 hrs  
 Statistical methods: The EL50 values were calculated by means of a parametric model developed by Kooijman [Kooijman, S.A.L.M. (1981) Parametric analyses of mortality rates in bioassays. Water Res. 15:105-119.]

**Test Conditions:** Test media were prepared by adding test material to 500 ml of fresh water (pH ~8, hardness ~210 mg CaCO<sub>3</sub> per liter) in a glass-stoppered conical flask and stirring for 4 hr before adding test animals (25/ flask). Test conditions: 20 °C; no aeration, food, replicate or media renewal. The test animals were less than 24 hr old at the start of the test, from a laboratory culture in standard fresh water. At

none of the dose levels was test substance visible during the test period. pH and oxygen were monitored. During the test, the oxygen concentration was >70% of the saturation level. The concentrations tested: 0, 3.2, and 10 mg/L (nominal).

<b>Results:</b>	EL <sub>50</sub> (48 hr) < 3.2 mg/L (estimated to be about 2) (EL0 <3.2 mg/L, EL10 = 10 mg/L) NOEC (48 hr) < 3.2 mg/L (nominal)
<b>Remarks:</b>	Assessment of condition of test animals compared to controls was by visual estimation.
<b>Reliability:</b>	(2) Reliable with restrictions. Study does not totally comply with current testing guidelines. No chemical analyses were performed.
<b>References:</b>	Adema, D.M.M. and Bakker, G.H. (1985) Aquatic toxicity of compounds that may be carried by ships [MARPOL 1973; Annex II]. TNO report R 85/217, The Hague (unpublished report).

#### 4.3 Toxicity to Aquatic Plants (e.g. Algae)

No data available.

#### 4.4 Toxicity to Micro-organisms, e.g. Bacteria

No data available

#### 4.5 Chronic Toxicity to Aquatic Organisms

##### A. Chronic Toxicity to Fish

<b>Test Substance:</b>	CAS No. 27215-95-8, Nonene; or CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich
<b>Method/Guideline:</b>	
Type (test type):	30-day Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000)
Species:	Fish
<b>Test Conditions:</b>	The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the

estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used Kow values of 4.55 for nonene and 4.62 for Alkenes, C8-10, C9 Rich. The Kow values were estimated by EPIWIN using the structure for 2-nonene for nonene and 1-nonene for the C9 Rich substance.

**Results:**

**Units/Value:** Estimated 30-day ChV for nonene = 73 µg/L  
Estimated 30-day ChV for Alkenes, C8-10, C9 Rich = 63 µg/L

**Flag:** Key study for SIDS endpoint

**Reliability:** (2) Reliable with restrictions. The result is calculated data.

**Reference:** EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Chronic Toxicity to Invertebrates**

**Test Substance:** CAS No. 27215-95-8, Nonene; or CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

**Method/Guideline:**

**Type (test type):** 16-day EC50 value calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000)

**Species:** *Daphnia magna*

**Test Conditions:** The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used Kow values of 4.55 for nonene and 4.62 for Alkenes, C8-10, C9 Rich. The Kow values were estimated by EPIWIN using the structure for 2-nonene for nonene and 1-nonene for the C9 Rich substance.

**Results:**

**Units/Value:** Estimated 16-day EC50 for nonene = 75 µg/L  
Estimated 16-day EC50 for Alkenes, C8-10, C9 Rich = 67 µg/L

**Flag:** Key study for SIDS endpoint

**Reliability:** (2) Reliable with restrictions. The result is calculated data.

**Reference:** EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### 4.6 Toxicity to Terrestrial Organisms

##### A. Toxicity to Terrestrial Plants.

**Test Substance:** CAS No. 27215-95-8, Nonene ; or CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

**Method/Guideline:**

**Type (test type):** 96-hr Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000)

**Species:** Green algae

**Test Conditions:** The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used Kow values of 4.55 for nonene and 4.62 for Alkenes, C8-10, C9 Rich. The Kow values were estimated by EPIWIN using the structure for 2-nonene for nonene and 1-nonene for the C9 Rich substance.

**Results:**

**Units/Value:** Estimated 96-hr ChV for nonene = 152 µg/L  
Estimated 96-hr ChV for Alkenes, C8-10, C9 Rich = 137 µg/L

**Flag:** Key study for SIDS endpoint

**Reliability:** (2) Reliable with restrictions. The result is calculated data.

**Reference:** EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.



**B. Toxicity to Soil Dwelling Organisms.**

No data available

**C. Toxicity to Other Non Mammalian Terrestrial Species (including Avian)**

No data available

**4.7 Biological Effects Monitoring (including Biomagnification)**

No data available

**4.8 Biotransformation and Kinetics**

No data available

**5. MAMMALIAN TOXICITY**

**5.1 Toxicokinetics, Metabolism and Distribution**

**A. Test Substance:** CAS No. 111-66-0, 1-Octene, >99%; CAS No. 124-11-8, 1-Nonene, >99%; CAS No. 872-05-9, 1-Decene, >98% (tested individually)

<b>Method</b>	Non-standard
<b>Test Type</b>	in-vivo
<b>GLP</b>	No data
<b>Year</b>	No data

**Method:** Animals were exposed via inhalation to individual hydrocarbons in 6 separate experiments with equal design except for the choice of test substance. Animals were killed by decapitation, and blood and organ samples were obtained within 3 minutes after removal of an animal from the chamber. Food and water were available *ad libitum* except during exposure. Dynamic exposure of the animals was performed in 0.7 m<sup>3</sup> steel chambers. Temperature and humidity were kept within 23±1°C and 70±20% RH, respectively. The aimed concentration of 100 ppm was maintained by mixing a controlled stream of air saturated with the test substance under a constant temperature and flow with the main stream of dust filtered air (5 m<sup>3</sup>/hr) before entering at the top of the chamber. The concentration of hydrocarbons in the chambers was monitored by on-line gas chromatography at 15 minute intervals. The concentration of hydrocarbons in tissues was determined by headspace gas chromatography. Two ml of blood or organ homogenate (or 0.25 g perirenal fat tissue) was equilibrated in 15 ml headspace vials for 1 hr at 37 or 60 °C together with calibration samples and blanks. 0.5 ml was

taken from the headspace by prewarmed gas tight syringe and injected into a Shimadzu GC 9A gas chromatograph (FID). Separation was performed on a 2 m x 1/8" stainless steel column packed with GP 10% SP-2100 on Supelcoport 100/120 mesh with nitrogen as carrier gas. In blood, the calibration curves covered a range from 0.5 – 100 µmol/kg, in organs from 1 – 500 µmol/kg and in fat from 5 – 10000 µmol/kg. In blood and organs, the detection limits generally were within the range from 0.1 to 1 µmol/kg; in fat from 1 to 10 µmol/kg.

**Test Conditions:**

Species:	Rat
Strain:	Sprague-Dawley
Sex:	Male
Age:	No data
Bodyweight:	150 – 200 g at start of each experiment
Number of Animals:	4 per exposure
Route:	Inhalation
Dose(s) used:	100 ppm for 3 days, 12 hr/day
Statistical Methods:	None reported
Actual Dose(s):	For the 3 days exposure period, the mean chamber concentration was 99.3 ppm
Body Fluids Sampled:	Blood sampled at days 1, 2, and 3, immediately after exposure and 12 hr after exposure on day 3
Tissues Sampled:	Brain, liver, kidney, fat; sampled at days 1, 2, and 3, immediately after exposure and 12 hr after exposure on day 3

**Results:** No systematic increase or decrease in biological concentrations was observed during the exposure period except for fat. With the exception for the kidney, the concentration increased with increasing number of carbon atoms within each structure group. The organ concentrations generally exceeded blood by factors ranging from 3 to 10. The C9 and C10 1-alkenes showed an increased accumulation in fat during the 3 days exposure period, in contrast to the C8 1-alkene, where a saturation seemed to occur. In fat, the concentrations of all hydrocarbons were 4-20 times the concentrations found in other organs. The 1-alkenes demonstrated high concentrations in fat 12 hr after exposure. After the recovery period, these concentrations were 31, 46, and 66% for C8, C9 and C10 1-alkenes, respectively, of the concentrations on day 3.

Concentrations of individual 1-alkenes after the third daily 12 hr exposure to 100 ppm and after 12 hr recovery (n=4)<sup>a</sup>

	1-Octene		1-Nonene		1-Decene	
	After third exposure	After 12 hr recovery	After third exposure	After 12 hr recovery	After third exposure	After 12 hr recovery
Blood	12.4	0.1	15.9	0.4	16.4	0.7
Brain	69.7	0.5	116.3	2.7	138.1	6.3
Liver	78.9	nd	130.4	1.1	192.8	4.0
Kidney	139.3	0.9	146.7	4.6	162.0	9.3
Fat	720	226	2068	953	2986	1971

<sup>a</sup> All concentrations are in  $\mu\text{mol/kg}$ ; nd = not detectable (limit of detection varied between substances and organs: in blood and organs generally within range from 0.1 – 1  $\mu\text{mol/kg}$ ; in fat from 5 – 10  $\mu\text{mol/kg}$ )

**Reliability:** (1) Reliable without restrictions.

**Reference:** Zahlse, K., I. Eide, A.M. Nilsen and O.G. Nilsen (1993) Inhalation kinetics of C8-C10 1-alkenes and iso-alkanes in the rat after repeated exposures. *Pharmacology & Toxicology* 73:163-168.

**B. Test Substance:** CAS No. 592-76-7, 1-Heptene ; CAS No. 2216-38-8, 2-Nonene; CAS No. 592-47-2, 3-Hexene; CAS No. 16746-85-3, 4-Ethyl-1-Hexene; CAS No. 15870-10-7, 2-Methyl-1-Heptene; CAS No. 3404-77-13, 3-dimethyl-1-hexene; 3-methyl-1-octene (tested individually)

**Method** Non-standard  
**Test Type** in-vitro and in-vivo  
**GLP** No data available  
**Year** Unknown

**Test Conditions:** In-vitro: Incubation of hepatic microsomes from rats in the presence of alkenes and NADPH with analysis for presence of cytochrome P-450.

In-vivo: Phenobarbital-treated rats were injected i.p. with 1-heptene, *cis* and *trans* 2-nonen, 4-ethyl-1-hexene, and 3-methyl-1-octene at a dose of 400  $\mu\text{l/kg}$ . Four hrs after treatment, animals were sacrificed and livers were analyzed for the presence of abnormal hepatic pigments. These pigments have been shown to be porphyrins derived from the prosthetic heme moiety of inactivated P-450 enzymes.

**Results:** *In vitro*: Hepatic microsomal cytochrome P-450 was destroyed *in vitro*, in the presence of NADPH, by 4-ethyl-1-hexene, 3-methyl-1-octene, and 1-heptene. The *cis*- and *trans*-2-nonenes exhibited marginal destructive activity (10% loss after 30 minutes). No significant cytochrome P-450 loss was observed after incubation with 2-methyl-1-heptene, 3,3-

dimethyl-1-hexene or 3-hexene, suggesting that steric and electronic factors can suppress the destructive interaction. The epoxides of 3 of the terminal olefin substrates were synthesized and shown not to intervene in destruction of the enzyme by the parent olefins.

*In vivo:* Hepatic green pigments were formed after administration of 4-ethyl-1-hexene, 3-methyl-1-octene and 1-heptene, indicating destruction of the P-450 enzyme. The cis- and trans-2-nonenenes produced no abnormal pigments.

**Reliability:** (1) Reliable without restrictions

**Reference:** Ortiz de Montellano, P.R., and Mico, G.A. (1980) Destruction of cytochrome P-450 by ethylene and other olefins. *Mol. Pharmacol.* 18(1)128-135.

## 5.2 Acute Toxicity

### A. Acute oral toxicity

#### Test Substance

Identity (purity): CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

#### Method

Method/guideline: NA  
Type (*test type*): LD50  
GLP: Pre-GLP  
Year: 1957  
Species/Strain: Holtzman Rat  
Sex: Males  
No. of animals per sex per dose: 5

Vehicle: 0.5% aqueous methyl cellulose solution  
Route of administration: Oral gavage

**Test Conditions:** Dose levels tested were 10.0, 31.6, 100, 316, 1000, and 3160  $\mu\text{l/kg}$  of body weight. The test material was administered as a 0.1, 1.0, or 10% volume/volume suspension in a 0.5% aqueous methyl cellulose solution. The by-weight equivalent doses were 7.4, 23.3, 73.8, 233, 738, and 2332 mg/kg. For the purpose of this study, the test material was considered to be free of impurities. Age of the test animals was not reported. Body weights ranged from 104 to 117g at initiation of the study. Control group and Treatment: For comparison, untreated animals were necropsied at the end of the study. Prior to dosage, food was withheld from the animals for three hours. Following exposure, food and water

were available at all times. The animals were observed for gross effects and mortality several times on the day of exposure and once daily thereafter for 7 days. Gross necropsies were performed at the end of the observation period. The statistics used to analyze the data were not reported.

**Results:**

Value: LD50 > 2332 mg/kg  
Number of deaths  
at each dose level: There were no deaths

Remarks: Animals in the high dose group appeared slightly depressed the day after administration of the test material. For several hours following exposure, the animals in the high dose group also showed slight nasal discharge. Otherwise, all animals appeared normal throughout the study. Animals in all groups exhibited normal weight gain. Gross necropsy did not reveal any abnormalities other than slightly congested adrenal glands in animals from the three higher dose levels (233, 738, and 2332 mg/kg). Under the conditions of this study, Alkenes, C8-10, C9 rich have a low order of toxicity.

**Reliability:** (1) Reliable without restrictions, comparable to a guideline study

**Flag:** Key study for SIDS endpoint.

**References:** Hazleton Laboratories for Esso Research and Engineering Co. (1957)  
Acute Oral Administration (unpublished report).

**B. Acute inhalation toxicity**

**Test Substance**

Identity (purity): CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

**Method**

Method/guideline: NA  
Type (*test type*): Inhalation LC50  
GLP: Pre-GLP  
Year: 1977  
Species/Strain: CD-1 Mice, Sprague-Dawley Rats, and Hartley Guinea Pigs  
Sex: Males and females  
No. of animals  
per sex: 5/species  
Vehicle: None  
Route of  
administration: Inhalation (vapor )

**Test Conditions:** For the purpose of this study, the test material was considered to be free of impurities. Age of the test animals was not reported. Body weights ranged from 24 to 32 g (mice), 228 to 321 g (rats), and 345 to 395 g (guinea pigs) at initiation of the study. Animals were given a single dose of test substance vapor at a concentration of 11.1 mg/L (2150 ppm) for 6 hours. An airstream was bubbled through the test material at a rate of 33.1 L/min and passed through a 760 L test chamber containing the test animals for a total of 6 hours. Control animals (5/sex/species) were exposed to clean air at the same flow rate as the treated group. Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Body weights were recorded on Days 0, 1, 2, 4, 7, and 14. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study. The statistics used to analyze the data were not reported.

**Results:**

**Value:** LC50 > 11.1 mg/L (2150 ppm) for 6 h for rats, mice and guinea pigs  
**Number of deaths at each dose level:** None of the animals died during the exposure period or during the 14-day post-exposure observation period.

**Remarks:** A total of 132.1 g of test material was delivered to the chamber during the course of the exposure. The overall nominal concentration of the test substance was 11.1 mg/L. During the last 4 hours of exposure, mice exhibited labored breathing patterns, rats exhibited limb ataxia and generally lethargic behavior, and the guinea pigs showed slight tremors. No similar signs were noted in the control animals, indicating that these effects were due to exposure to the test substance. However, all of the symptoms subsided as the test chamber was cleared with clean air. On day 4 of the post-exposure observation period, one of the exposed mice had tremors, but the symptoms only occurred on that day and were not believed to be due to exposure to the test substance. Signs of toxicity observed during the 14-day post-exposure period included dry rales, soft stool, and nasal discharge in rats, however, these signs were observed in both the exposed and control animals and are not believed to be due to the test substance. In both exposed animals and controls, there was a slight decrease in body weight during the first few days following exposure, after which the animals recovered their normal body weight. There were no significant differences observed between the exposed animals and the test animals at necropsy. Although there was a high incidence of kidney lesions in both groups of guinea pigs, the rate was slightly higher in the exposed animals than in the controls. However, the difference was not statistically significant.

Under conditions of this study, Alkenes, C8-10, C9 rich have a low order of acute inhalation toxicity in rats.

**Reliability:** (1) Reliable without restrictions; comparable to a guideline study.

**Flag:** Key study for SIDS endpoint

**References:** Bio/dynamics, Inc. (1977) An Acute Inhalation Toxicity Study of MRD-76-57 in the Mouse, Rat, and Guinea Pig. Conducted for Exxon Research and Engineering Company (unpublished report).

### C. Acute dermal toxicity

#### Test Substance

Identity (purity): CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

#### Method

Method/guideline: NA  
 Type (*test type*): LD50  
 GLP: Pre-GLP  
 Year: 1957  
 Species/Strain: Albino rabbits  
 Sex: Males  
 No. of animals per sex per dose: 4

Vehicle: NA  
 Route of administration: Dermal

**Test Conditions:** For the purpose of this study, the test material was considered to be free of impurities. Age of the test animals was not reported. Body weights ranged from 1.4 to 2.2 kg at initiation of the study. Animals received single 24-hr exposures to test substance at concentration levels of 73.8, 233, 738, and 2332 mg/kg. There was no control group. Undiluted test material was applied to clipped, intact abdominal skin under rubber dental damming. The trunks of the animals were wrapped securely with adhesive binder to prevent ingestion of the test substance. Following the 24-hour exposure period, the binder was removed and the exposed area was sponged with warm water to remove residue. Animals were observed for gross signs of irritation and systemic toxicity daily for 7 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually. The statistics used to analyze the data were not reported.

#### Results:

Value: LD50 > 2332 mg/kg  
 Number of deaths at each dose level: No mortalities were observed at any dose tested.

**Remarks:** The abdomens and binders were dry at the end of the exposure period, indicating a good rate of dermal absorption of the applied material. The test material produced mild dermal irritation characterized by mild erythema. Most of the animals showed slight atonia for several days of the observation period and desquamation during the final two days of the observation period. Throughout the study, all animals exhibited normal appearance and behavior. Body weight gain was normal throughout the study. There were no significant findings at necropsy. Alkenes, C8-10, C9 rich have a low order of acute dermal toxicity.

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint

**References:** Hazleton Laboratories for Esso Research and Engineering Co. (1957) Acute Dermal Application (unpublished report).

**D. Acute toxicity, other routes**

No data available

**5.3 Corrosiveness/Irritation**

**A. Skin Irritation/Corrosion**

**Test Substance**

**Identity (purity):** CAS No. 68526-55-6; Alkenes, C8-10, C9 rich

**Method**

**Method/guideline:** NA  
**Type (test type):** Dermal irritation  
**GLP:** Pre-GLP  
**Year:** 1957  
**Species/Strain:** Albino rabbits  
**Sex:** Males  
**No. of animals per sex per dose:** 4

**Vehicle:** NA  
**Route of administration:** Dermal

**Test Conditions:** Animals received single 24-hr exposures to test substance at concentration levels of 73.8, 233, 738, and 2332 mg/kg. There was no control group. Undiluted test material was applied to clipped, intact abdominal skin under rubber dental damming. The trunks of the animals were wrapped securely with adhesive binder to prevent ingestion of the



test substance. Following the 24-hour exposure period, the binder was removed and the exposed area was sponged with warm water to remove residue. Animals were observed for gross signs of irritation and systemic toxicity daily for 7 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually.

Age of the test animals was not reported. Body weights ranged from 1.4 to 2.2 kg at initiation of the study. The statistics used to analyze the data were not reported

**Results:**

Number of deaths  
at each dose level:

No mortalities were observed at any dose tested.

Remarks:

The abdomens and binders were dry at the end of the exposure period, indicating a good rate of dermal absorption of the applied material. The test material produced mild dermal irritation characterized by mild erythema. Most of the animals showed slight atonia for several days of the observation period and desquamation during the final two days of the observation period. Throughout the study, all animals exhibited normal appearance and behavior. Body weight gain was normal throughout the study. There were no significant findings at necropsy.

**Reliability:**

(1) Reliable without restrictions

**References:**

Hazleton Laboratories for Esso Research and Engineering Co. (1957)  
Acute Dermal Application (unpublished report).

**B. Eye Irritation/Corrosion**

**Test Substance**

Identity (purity): CAS No. 68526-55-6; Alkenes, C8-10, C9 rich

**Method**

Method/guideline: Not specified  
Type (*test type*): Ocular irritation  
GLP: Pre-GLP  
Year: 1962  
Species/Strain: Albino rabbits  
Sex: Males and females  
No. of animals  
per dose: 6  
  
Vehicle: None  
Route of

administration: Ocular

**Test Conditions:** The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the left eye of each animal. The upper and lower lids were gently held together briefly to insure adequate distribution of the test material. The contralateral eye in each rabbit served as the control. Throughout the study, food and water were available at all times and animals were housed individually. The age and weight of the test animals was not reported. Statistics used to evaluate the data were not reported.

The general health of each rabbit was examined for irritation of the cornea, iris and conjunctiva at 1 and 4 hours and on days 1, 2, 3, 4 and 7. Ocular reactions were graded according to the Draize Standard Eye Irritation Grading Scale.

**Results:** Maximum total Draize score = 6

**Remarks:** There were no animal deaths prior to study termination. The test material produced mild conjunctival irritation which completely cleared within 24 hours.

**Reliability:** (1) Reliable without restrictions

**References:** Hazleton Laboratories for Esso Research and Engineering Co. (1962) Acute Eye Application - Rabbits (unpublished report).

#### 5.4 Skin Sensitisation

No data available

#### 5.5 Repeated Dose Toxicity

No data available

#### 5.6 Genetic Toxicity *in vitro*

##### A. Gene Mutation

###### Test Substance

Identity (*purity*): CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

###### Method

Method/guideline: EPA OTS 798.5265  
Type: in-vitro bacterial reverse mutation – Ames Assay  
System of testing: bacterial  
GLP: Yes

Year: 1991  
Species/Strain: *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538  
Metabolic activation: With and without S9 fraction of livers from rats pretreated with Aroclor 1254

Concentrations tested: 10, 32, 100, 320 and 1000 µg/plate (Doses were based on a pre-test for toxicity)

Statistical Methods: The mean plate count and standard deviation for each dose point were determined. Any test value that was equal to or greater than three times the mean value of the concurrent vehicle control was considered to be a positive dose.

**Test Conditions:** For the purpose of this study, the test material was considered to be free of impurities. DMSO was the vehicle for controls. Ethanol was the vehicle for the test material. Vehicle controls were dosed at 0.1 ml/plate ethanol and 0.1 ml/plate DMSO. The positive controls were 2-Aminoanthracene, 9-Aminoacridine, 2-Nitrofluorene, N-methyl-N-nitro-N-nitrosoguanidine. Three plates were prepared for each dose level.

To determine the highest dose of compound to be used in the assay, a dose range from 1 to 10,000 µg/plate was tested. Only strain TA98 was used. The toxicity pretest was repeated and toxicity was observed as a reduction in both background and revertant colony counts. 1000 µg/plate was selected as the high dose to be used on the mutagenesis assay for both the saline (-S9) and the +S9 treated plates.

A repeat assay was performed in order to verify the data produced in the initial assay.

## Results

Cytotoxic conc.: 1000 µg/plate  
Genotoxic effects: Negative with and without metabolic activation

Remarks: The test material did not produce any evidence of mutagenicity. In the initial and repeat assays, neither a positive response nor a dose related increase in revertants was observed for any of the tester strains either in the presence or absence of metabolic activation. All positive and negative controls responded in a manner consistent with data from previous assays. Under conditions of this assay, the test material was not mutagenic for the *Salmonella* tester strains at doses up to and including 1000 µg/plate.

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint.

**References:** Exxon Biomedical Sciences, Inc. (1991) Microbial Mutagenesis in *Salmonella*: Mammalian Microsome Plate Incorporation Assay (unpublished report).

**B. Chromosomal Aberration**

No data available

**5.7 Genetic Toxicity *in vivo***

**Test Substance**

Identity (purity): CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

**Method**

Method/guideline: EPA OTS 798.5395  
Type: Micronucleus Assay  
GLP: Yes  
Year: 1991  
Species: Mouse  
Strain: B6C3F1  
Sex: Male and female  
Route of Administration: Oral gavage  
Concentration levels: 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study.  
Exposure period: Single dose  
Statistical methods: Analysis of variance (ANOVA), Duncan's Multiple Range Test; sexes were analyzed separately

**Test Conditions:** For the purpose of this study, the test material was considered to be free of impurities. The test animals were approximately 8 to 9 weeks of age and weighed between 21 and 29 g at the start of the study. The test material and the carrier (corn oil) were administered by oral gavage as single doses to 15 mice/sex/dose (not fasted). The positive control, cyclophosphamide, was administered by intraperitoneal injection as a single dose of 40 mg/kg in reagent grade water at the same volume as the test material. Animals from the appropriate groups (5 animals/sex/group) were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended in fetal bovine serum, and prepared for microscopy. Samples were blindly coded and stained with acridine orange. 1000 polychromatic erythrocytes (PCE) from each animal were examined for micronuclei, and the ratio of PCE's to NCE's (normochromatic erythrocytes) was determined for each animal by counting 1000 erythrocytes (PCE's and NCE's)

## Results

Effect on PCE/NCE ratio:	The test material induced a significant decrease in polychromatic erythrocytes in both males and females at 48 and 72 hours when treated with the high dose (5.0 g/kg). In addition, the mean percent of PCE's for the 5.0 g/kg dose group for both sexes at 48 and 72 hours were statistically different from the carrier controls. The mean percent of PCE's for the female 2.5 g/kg dose group at 48 hours was also statistically different from the carrier control.
Genotoxic effects:	Negative.
NOEL:	5.0 g/kg
Remarks:	There was no statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. Thus, the test material was not clastogenic. The positive control induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, which indicates that the positive control responded appropriately and is clastogenic. These observations indicate that the test material was toxic to mouse bone marrow at higher concentrations, but did not induce micronuclei formation. Under conditions of this assay, the test material is not considered clastogenic in mice up to and including 5.0 g/kg when evaluated up to 72 hours after dose administration.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Exxon Biomedical Sciences, Inc. (1991) In vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Method (unpublished report).

### 5.8 Carcinogenicity

No data available

### 5.9 Reproductive Toxicity (including Fertility and Developmental Toxicity).

#### A. Fertility

No data available

#### B. Developmental Toxicity

No data available

## 5.10 Other Relevant Information

### Aspiration

#### Test Substance

Identity: C6-C18 even numbered alpha olefins

#### Method

Type: General toxicity – aspiration

Species: Rat

Strain: Wistar

Sex: Male

Route of

Administration: aspiration

Dose: 0.2 mL

Results: See Remarks

Remarks: C6-C18 alkenes (even carbon numbers, alpha olefins), source and purity unspecified, were assessed for aspiration hazard in an animal study using Wistar rats. Four or five males were used per test article. Two-tenths mL of the test material was placed in the mouths of rats that had been anesthetized to the point of apnea in a covered wide mouth gallon jar containing about 1 inch of wood shavings moistened with approximately 1 ounce of anhydrous diethyl ether. As the animals began to breathe again, the nostrils were held until the test material had been aspirated or the animal regained consciousness. All alkenes tested except 1-hexene were aspirated into the lungs. 1-Hexene was difficult to dose because of its volatility. Two animals survived because the hydrocarbon “boiled” out of the mouth before it was aspirated. All animals exposed to C<sub>8</sub> to C<sub>14</sub> died within 24 hours. With C<sub>16</sub> and C<sub>18</sub>, there was only one death (C<sub>18</sub>). Lung weights were increased in alkenes-treated animals compared with controls. The affected animals showed chemical pneumonitis. The report concluded that there is a significant aspiration hazard with C<sub>6</sub> to C<sub>14</sub> alkenes.

Reference: Gerarde, H.W. (1963) Toxicological Studies on Hydrocarbons. Archives of Environmental Health 6:329-341.

Other: This study was included in the dossier for 1-decene at SIAM 11.

## 5.11 Experience with Human Exposure

No data available

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